Electronic Supplementary Material (ESI) for Journal of Materials Chemistry A.

Dynamical Stabilization in Delafossite Nitrides for Solar Energy Conversion

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Supplementary Material

Table S1: Standard deviation (σ_{oct}) of bond angles for B-N bonds in the octahedral coordinations of each compound, computed from the relaxed structure at 0 K.

Compound	B-N σ_{oct} (deg.)
$CuTaN_2$	7.09
$CuNbN_2$	7.02
$CuVN_2$	3.80
$AgTaN_2$	7.29
$AgNbN_2$	7.25
$AgVN_2$	4.89
$AuTaN_2$	7.23
$AuNbN_2$	7.18
$AuVN_2$	4.11

Table S2: Computed internal parameters are shown for $CuBN_2$, $AgBN_2$, and $AuBN_2$, where B = Ta, Nb, and V. Interchanging the B elements has no effect on the parameters. Values are of fractional coordinates u_1, u_2, and u_3.

Compound	Element	u_1	u_2	u_3
$CuBN_2$				
	B	2/3	1/3	5/6
	B	1/3	2/3	1/6
	B	0	0	1/2
	Cu	0	0	0
	Cu	2/3	1/3	1/3
	Cu	1/3	2/3	2/3
	N	0	0	0.894
	N	0	0	0.106
	N	2/3	1/3	0.227
	N	2/3	1/3	0.439
	N	1/3	2/3	0.561
	N	1/3	2/3	0.772
$AgBN_2$				
	B	2/3	1/3	5/6
	B	1/3	2/3	1/6
	B	0	0	1/2
	Ag	0	0	0
	Ag	2/3	1/3	1/3
	Ag	1/3	2/3	2/3
	N	0	0	0.889
	N	0	0	0.111
	N	2/3	1/3	0.222
	N	2/3	1/3	0.444
	N	1/3	2/3	0.556
	N	1/3	2/3	0.778

$AuBN_2$				
	B	2/3	1/3	5/6
	B	1/3	2/3	1/6
	B	0	0	1/2
	Ag	0	0	0
	Ag	2/3	1/3	1/3
	Ag	1/3	2/3	2/3
	N	0	0	0.890
	N	0	0	0.110
	N	2/3	1/3	0.223
	N	2/3	1/3	0.443
	N	1/3	2/3	0.557
	N	1/3	2/3	0.777

Table S3: Values of full width at half maximum (FWHM) for the radial distribution functions of A-N and B-N pairs within each compound.

Compound	$FWHM_{A-N}$ (Å)	$FWHM_{B-N}$ (Å)
$CuTaN_2$	0.12	0.24
$CuNbN_2$	0.11	0.28
$CuVN_2$	0.13	0.31
$AgTaN_2$	0.15	0.24
$AgNbN_2$	0.13	0.28
$AgVN_2$	0.17	0.39
$AuTaN_2$	0.12	0.24
$AuNbN_2$	0.11	0.26
$AuVN_2$	0.13	0.34

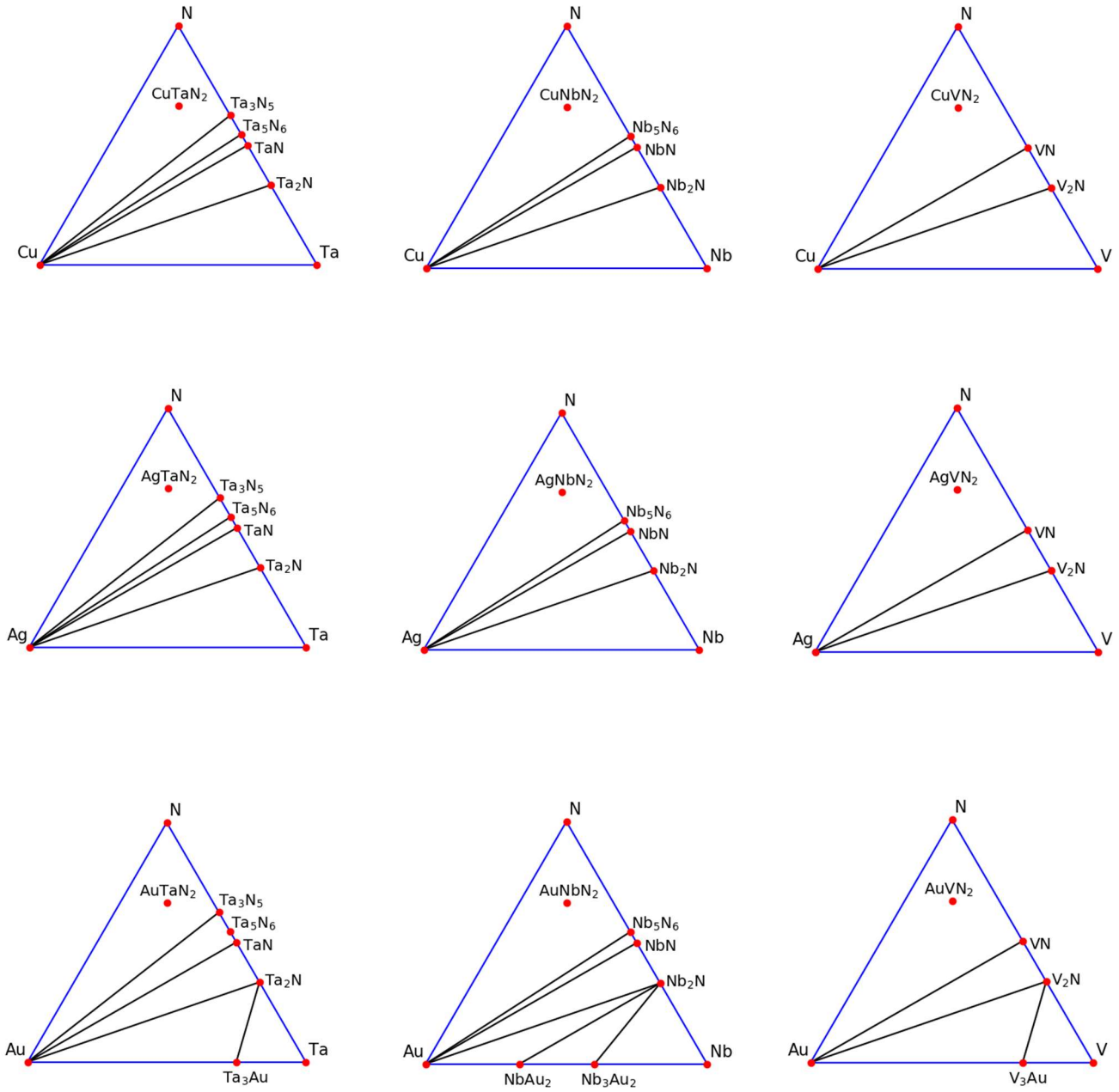


Figure S1: Diagrams showing all binaries considered when calculating ternary A-B-N convex hulls. In each case, ABN_2 lies above the hull.

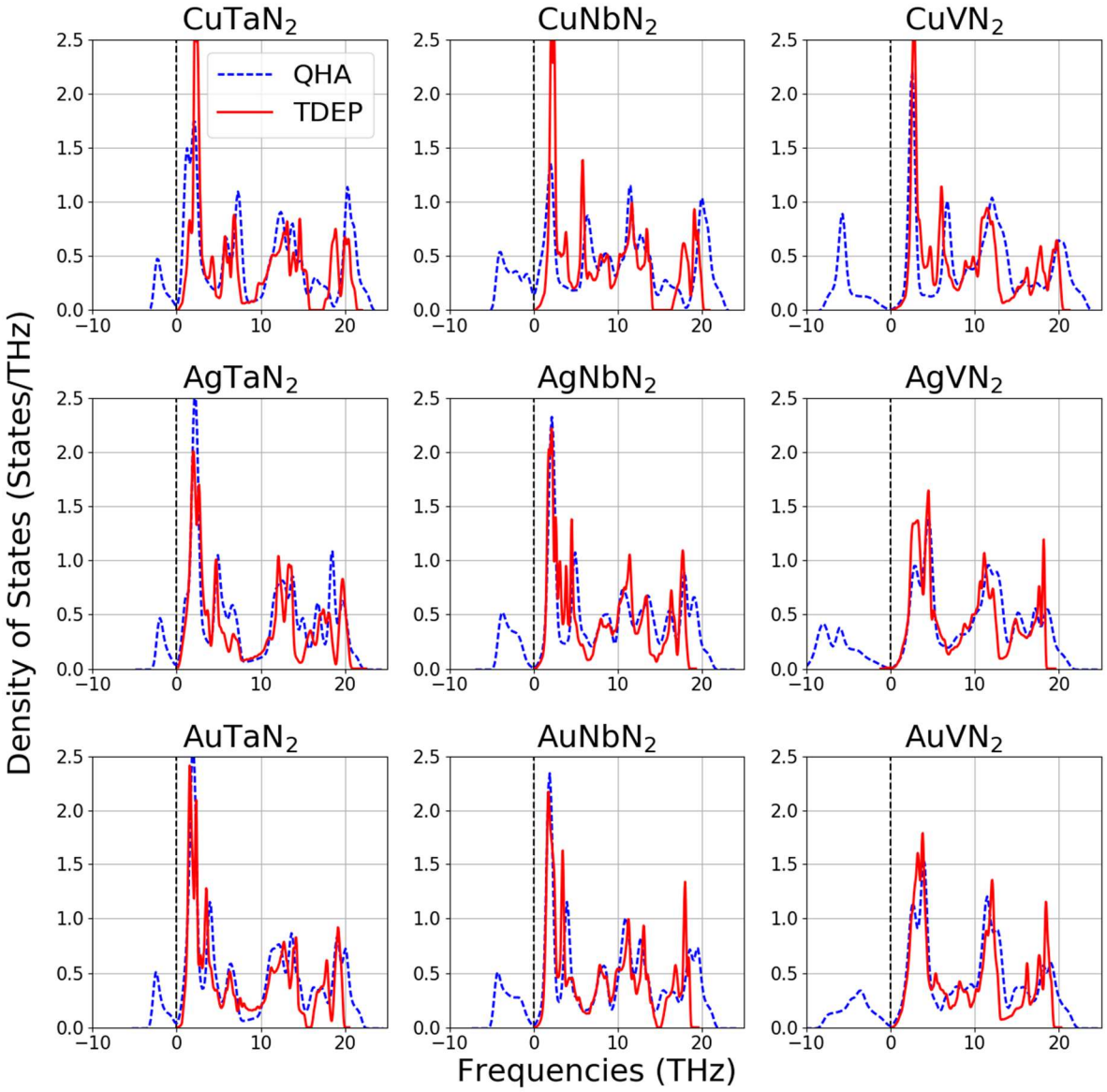


Figure S2: Phonon density, calculated using two unique methods: (i) QHA at 0 K and (ii) TDEP at 300 K. Densities are normalized per unit cell. The dashed vertical line represents zero frequency, separating positive (real) from negative (imaginary) frequencies.

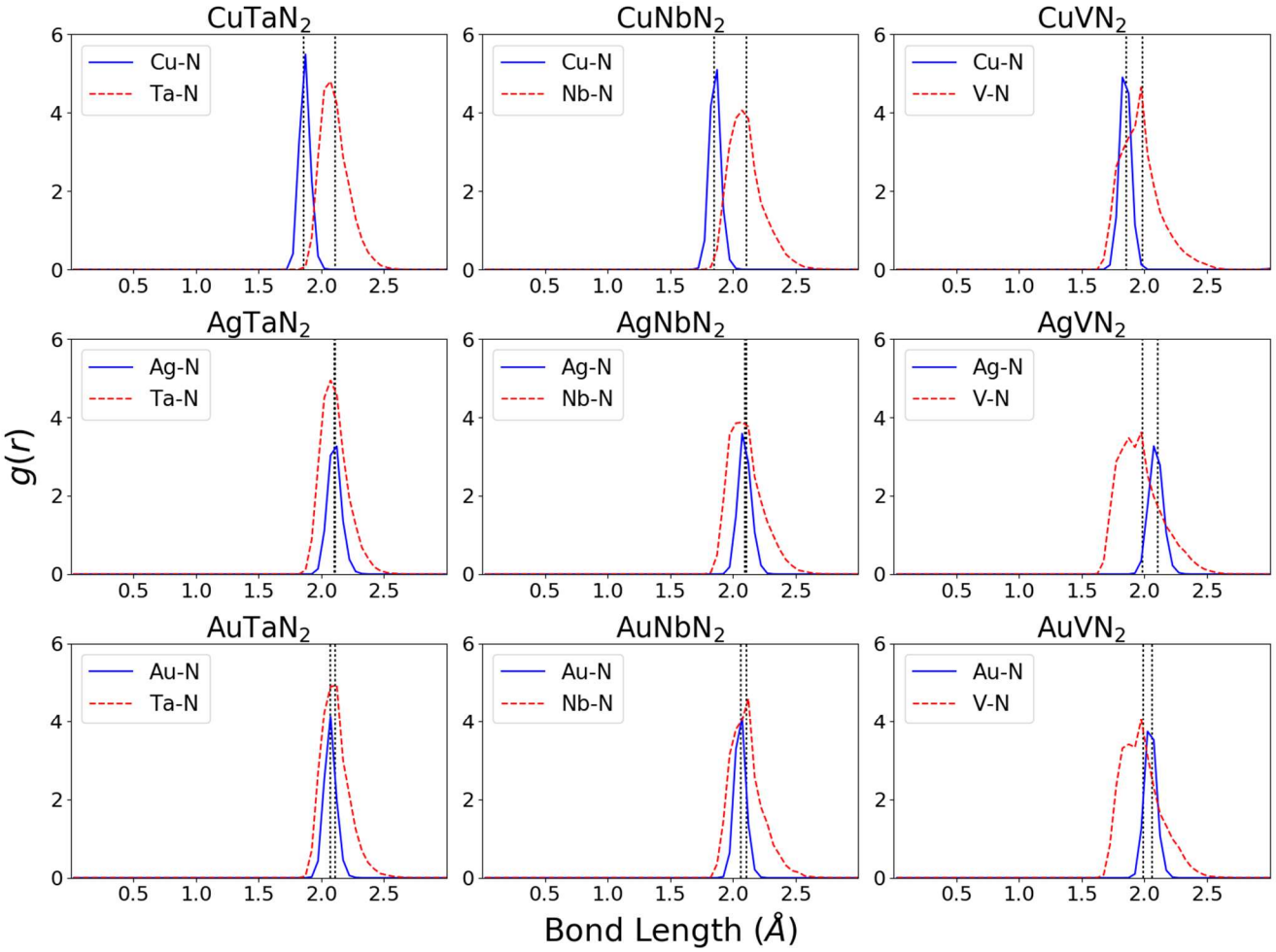


Figure S3: Radial distribution functions *g(r)* for A-N and B-N pairs within each compound, obtained using data from all 8,000 time steps of the molecular dynamics runs at 300 K. Equilibrium bond lengths are shown by dashed vertical lines.

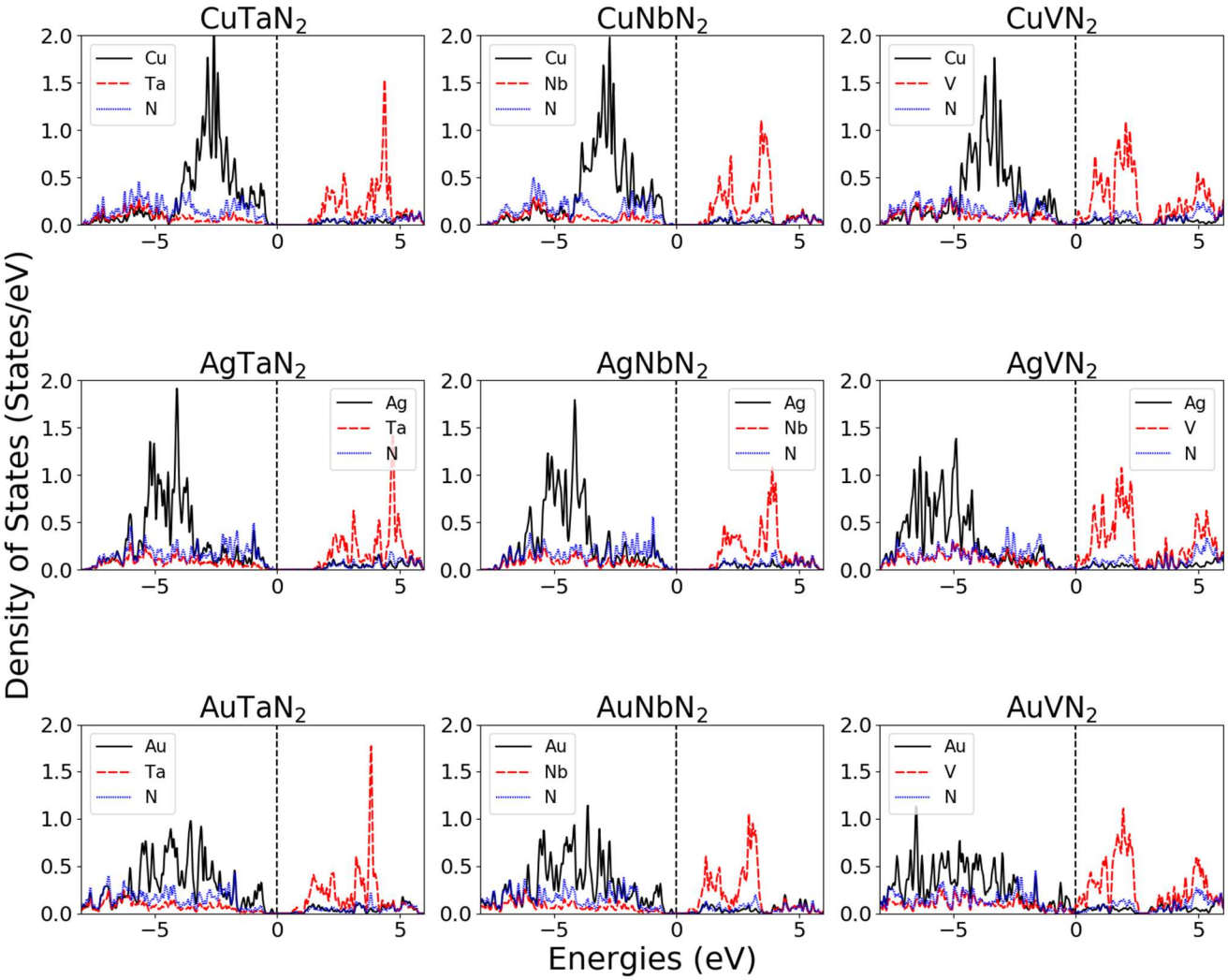
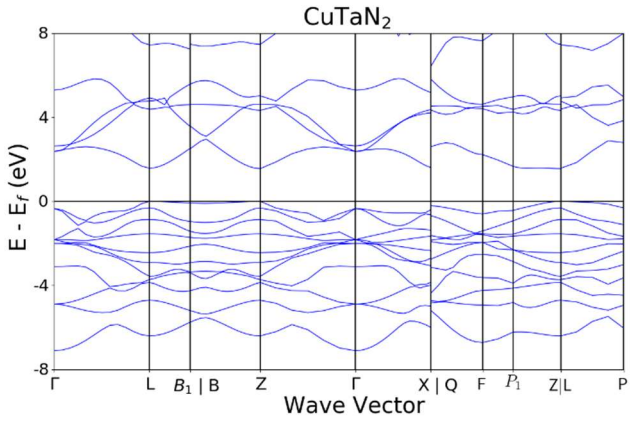
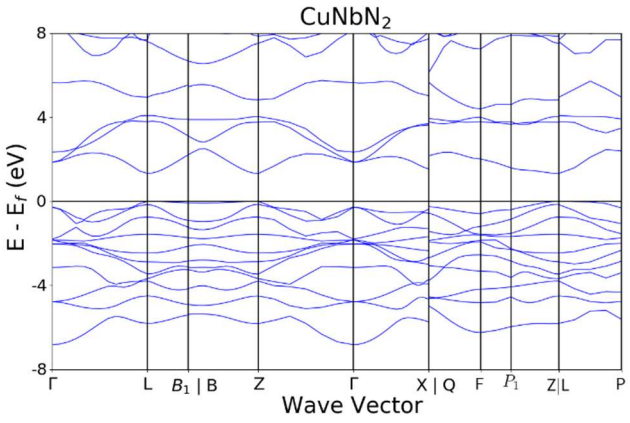
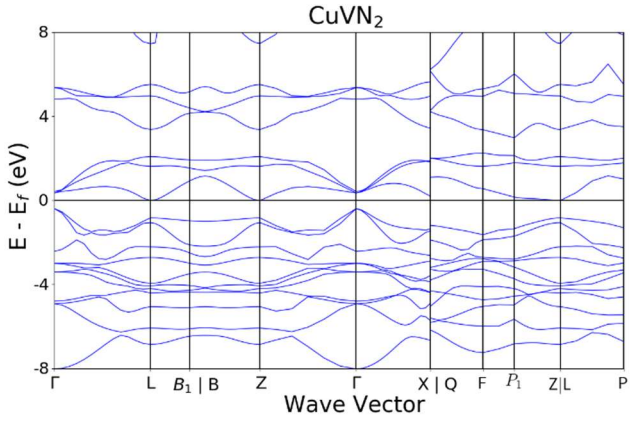
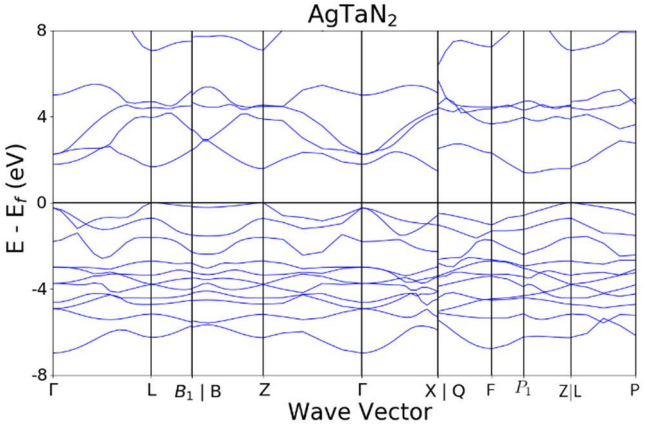


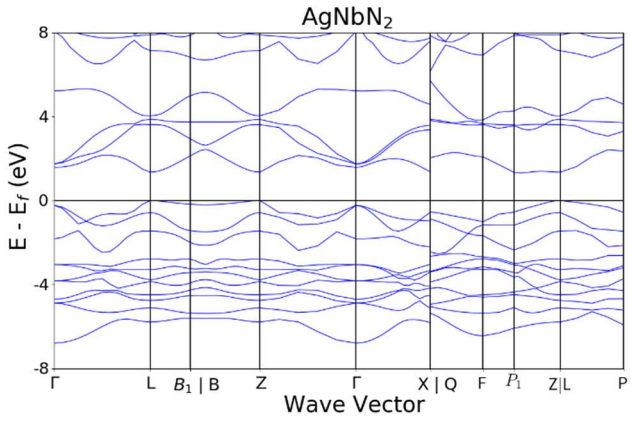
Figure S4: Electronic density of states for each compound, computed through implementation of the HSE06 functional. The densities are separated into their elemental components and are labeled as such. The Fermi energy is set to 0 eV.

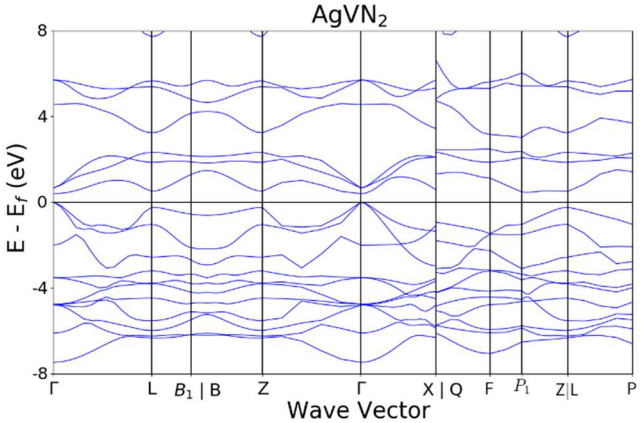

CuTaN2
E - Ef (eV)
8
4
0
-4
-8
Γ
L
B1 | B
Z
Γ
X | Q
F
P1
Z|L
P
Wave Vector


CuNbN2
E - Ef (eV)
8
4
0
-4
-8
Γ
L
B1 | B
Z
Γ
X | Q
F
P1
Z|L
P
Wave Vector


CuVN2
E - Ef (eV)
8
4
0
-4
-8
Γ
L
B1 | B
Z
Γ
X | Q
F
P1
Z|L
P
Wave Vector


AgTaN2
E - Ef (eV)
8
4
0
-4
-8
Γ
L
B1 | B
Z
Γ
X | Q
F
P1
Z|L
P
Wave Vector


AgNbN2
E - Ef (eV)
8
4
0
-4
-8
Γ
L
B1 | B
Z
Γ
X | Q
F
P1
Z|L
P
Wave Vector


AgVN2
E - Ef (eV)
8
4
0
-4
-8
Γ
L
B1 | B
Z
Γ
X | Q
F
P1
Z|L
P
Wave Vector

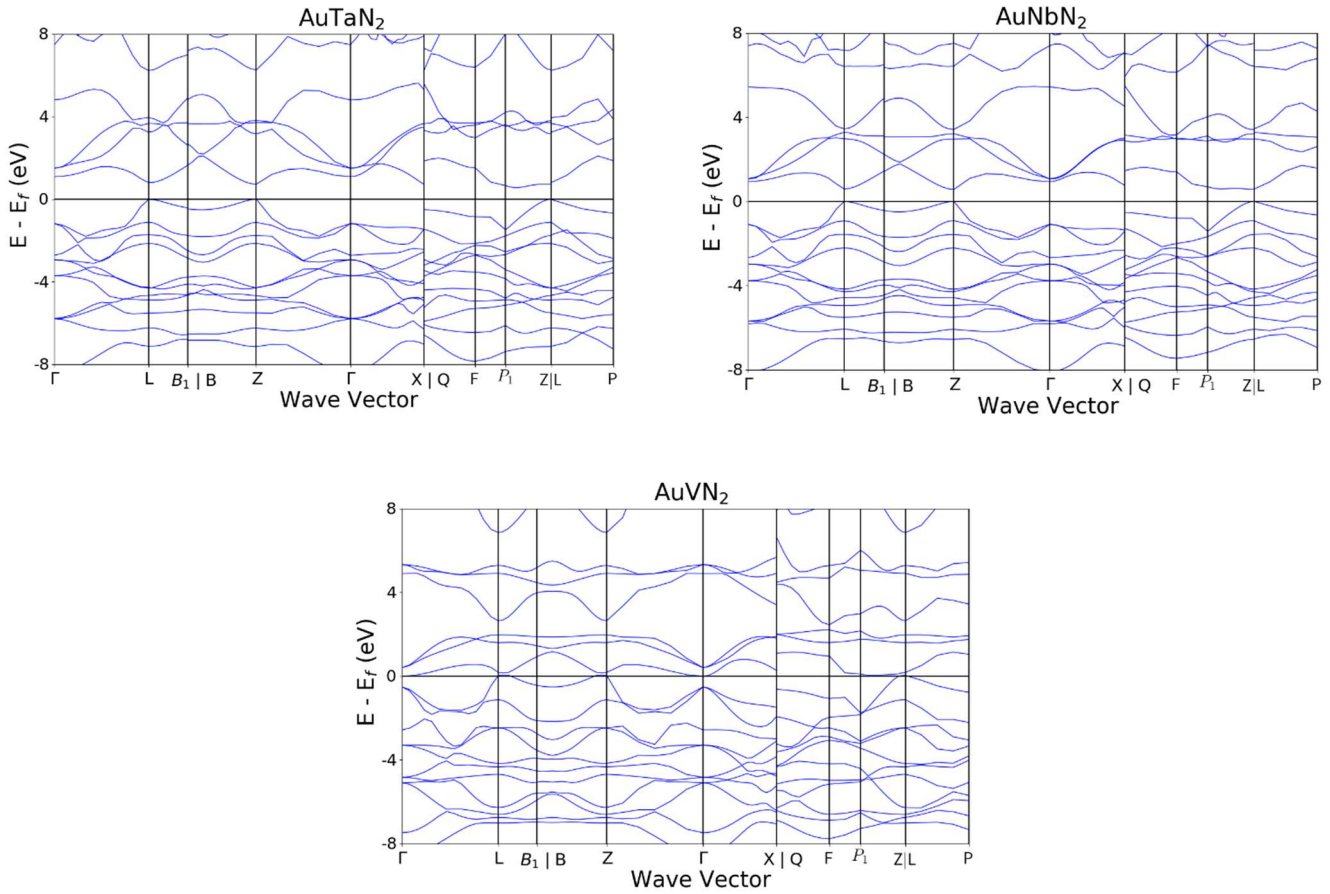


Figure S5: Electronic band structure along high-symmetry directions in the Brillouin zone. Fermi energy is set to 0 eV. All band gaps are indirect (*Z*-*L*).

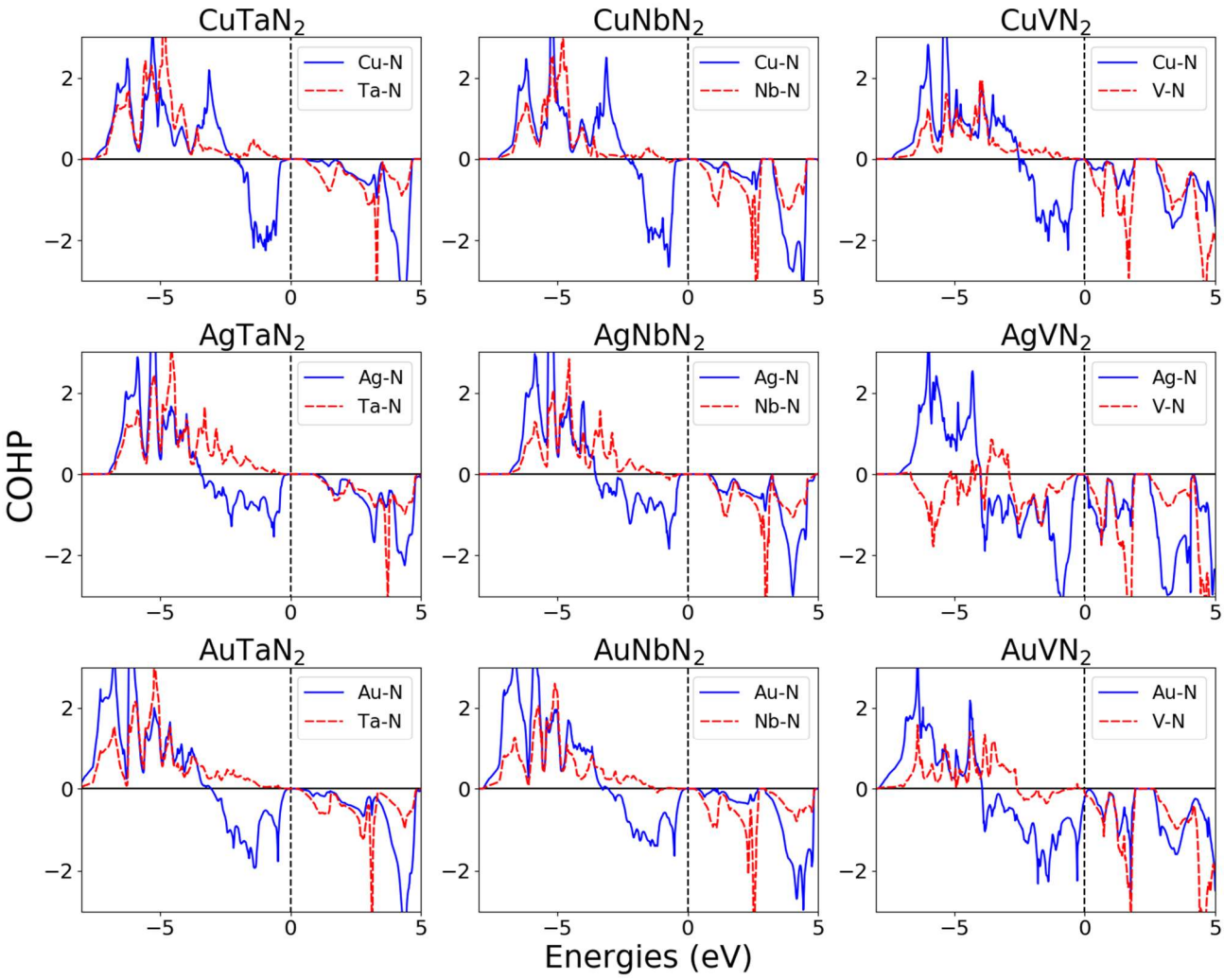


Figure S6: Crystal Orbital Hamiltonian Populations (COHP), separated into the two major bonding pairs: A-N and B-N. Other A-B and N-N populations are not shown here, as their magnitudes are insignificant compared to the A-N and B-N populations. Bonding states are assigned positive values while antibonding states are assigned negative values. The Fermi energy is set to 0 eV.

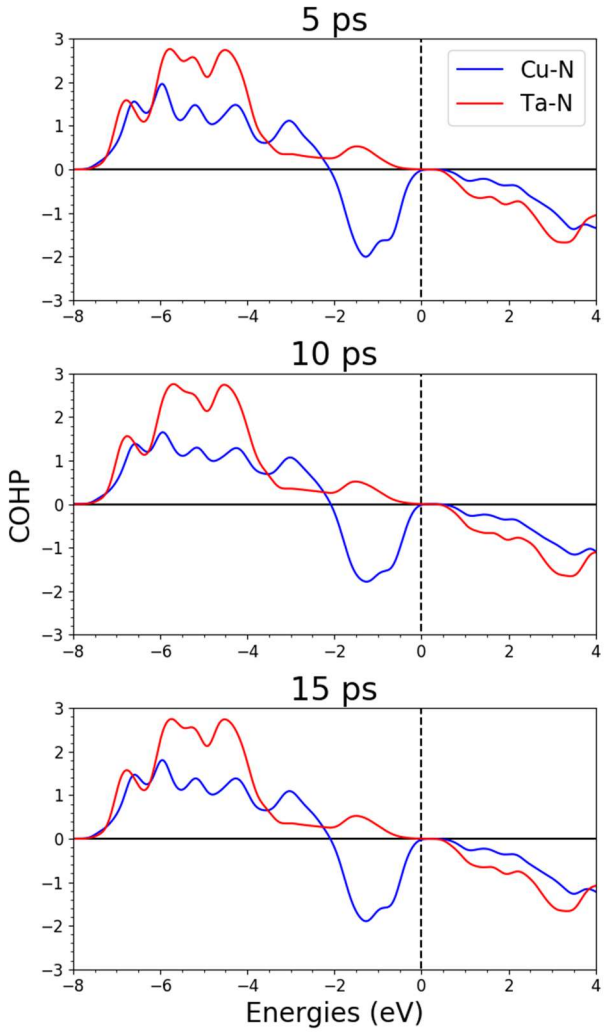


Figure S7: Crystal Orbital Hamiltonian Populations (COHP), separated into the two major bonding pairs: Cu-N and Ta-N. Bonding states are assigned positive values while antibonding states are assigned negative values. The Fermi energy is set to 0 eV. Structures are sampled from molecular dynamics calculations at three time steps: 5, 10, and 15 ps.

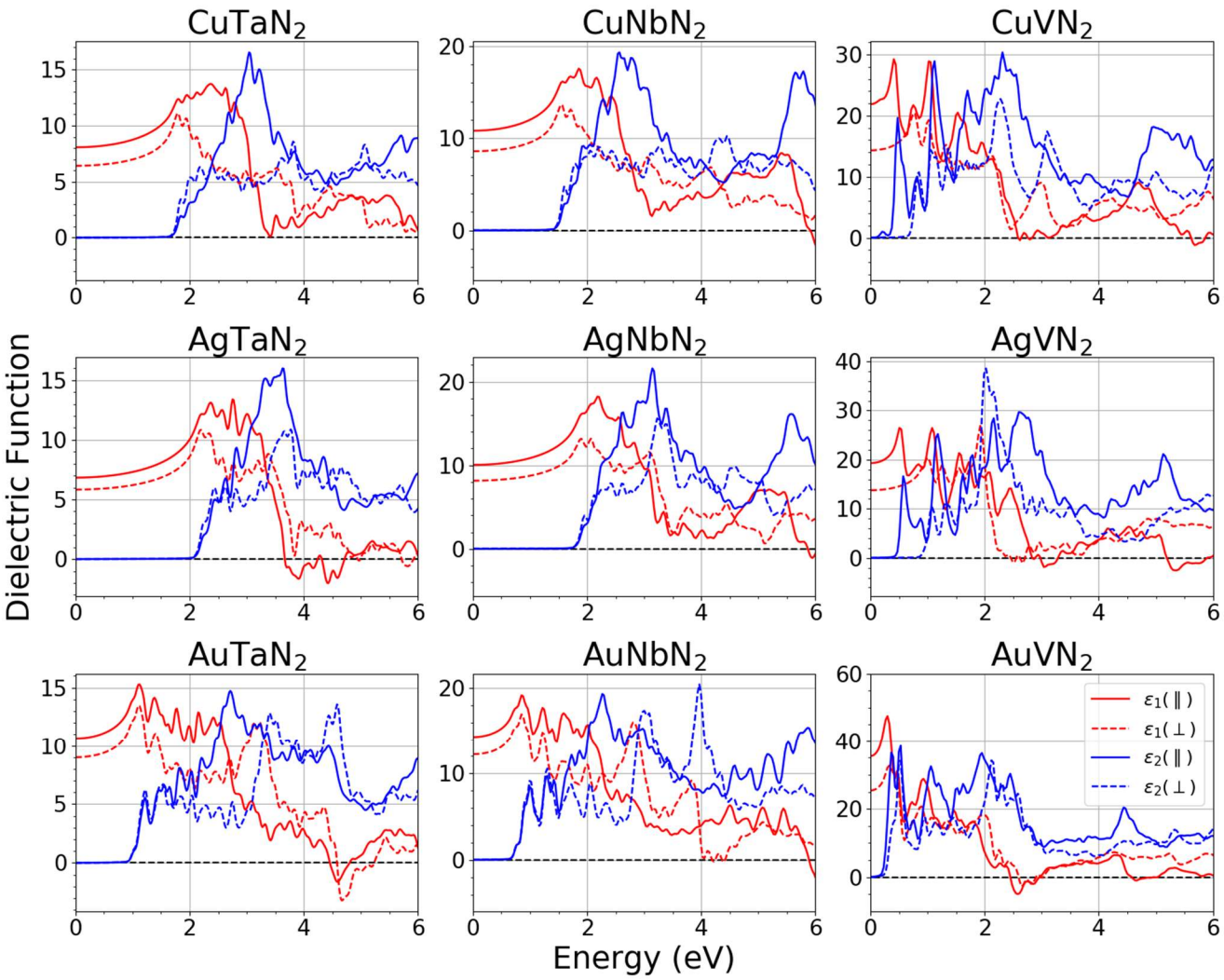


Figure S8: The real and imaginary parts of the complex dielectric function, computed through implementation of the hybrid HSE06 functional. The materials are anisotropic, such that the properties in the z-direction differ from those of the x- and y-direction. Therefore, the two independent directional values, parallel and perpendicular to the z-axis, are plotted for both ε_1 and ε_2.

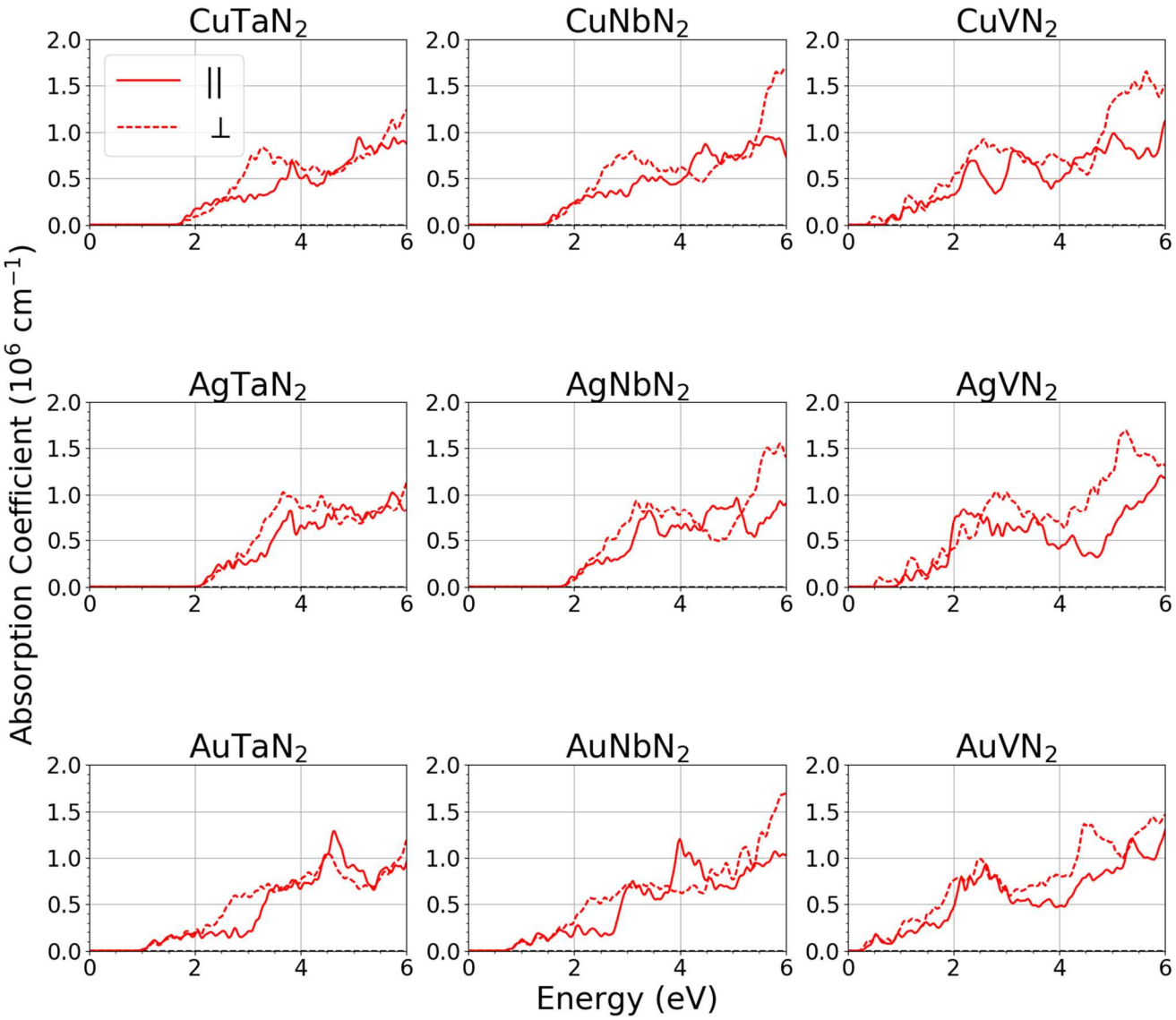


Figure S9: Absorption coefficients of each compound, computed through implementation of the hybrid HSE06 functional. The two independent directional values are plotted.